

USER

HOST

DEVICE

[run.sh]

gpue <args>

[main]

[parseArgs()]

Parse

arguments

[initialise()]

Setup host

Define **DEVICE** grid, block, and thread size

Calculate position and reciprocal space quantities

Allocate wavefunction, Hamiltonian, evolution operator memory blocks

Define initial wavefunction, Hamiltonian, evolution operators

[FileIO::writeOutXYZ()]

Write out to file

Open file and write

Free unnecessary memory

Allocate CUFFT plans

0

[FileIO::readIn()]

Read wavefunction from file

Open, read and write data to memory

wfc-Copy **HOST** memory values to **DEVICE** memory-

[evolve]

Perform
evolution

Initialise simulation variables

Print wavefunction at defined timesteps

Evolution loop

[Tracker::vortPos()]

Track vortex
position to nearest grid pointLocate +/- 2Pi
phase windings**vortCoords**

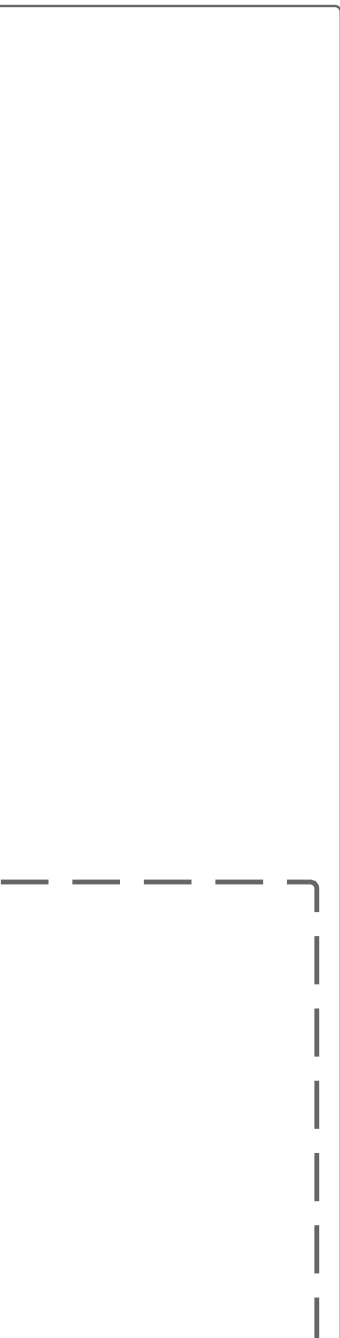
[Tracker::lsFit()]

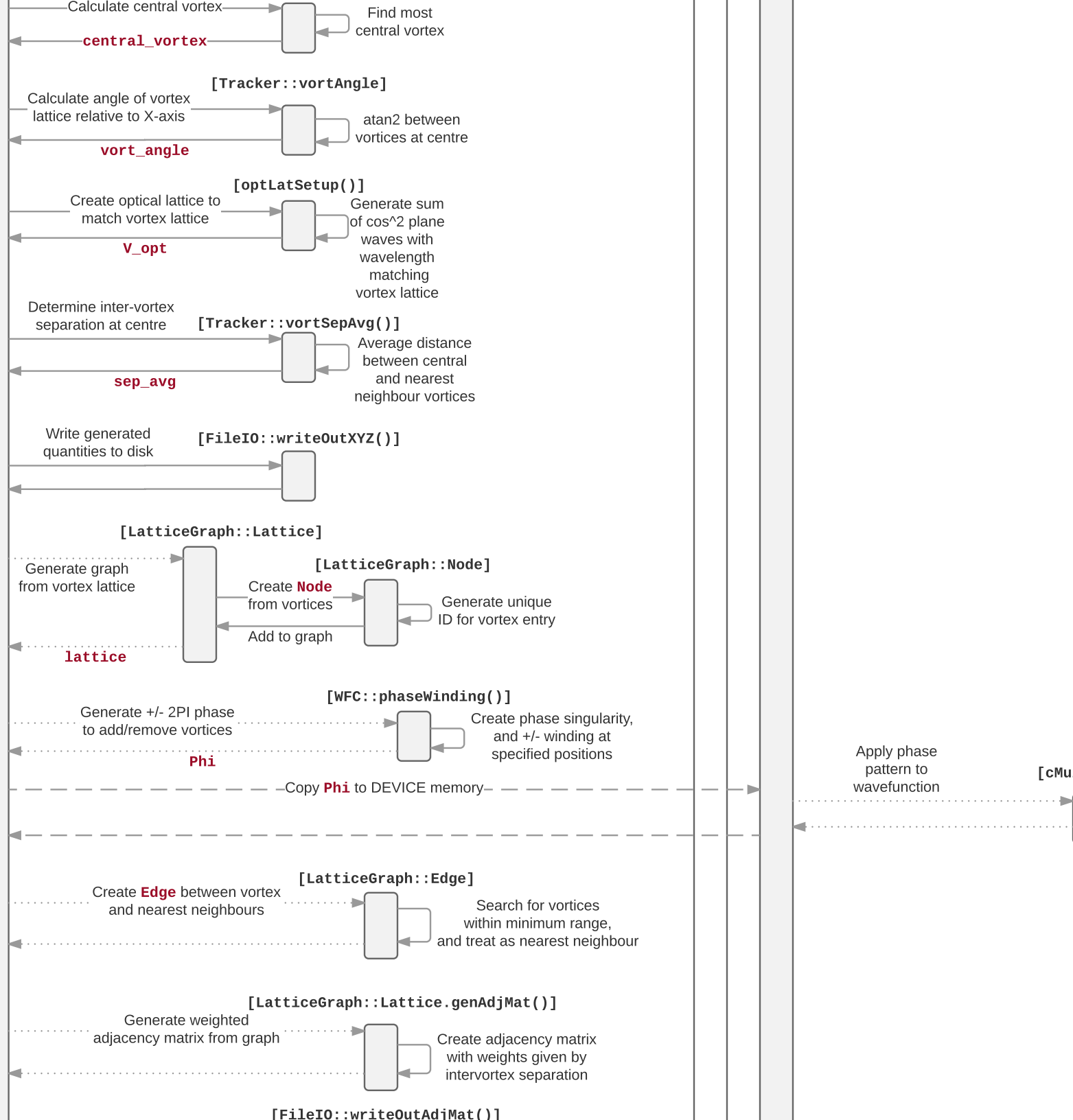
Calculate accurate vortex
position with least squaresUse 2x2 grid
plaquettes
to determine
vortex position**vortCoords**

[Tracker::vortCentre()]

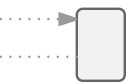
Calculate central vortex

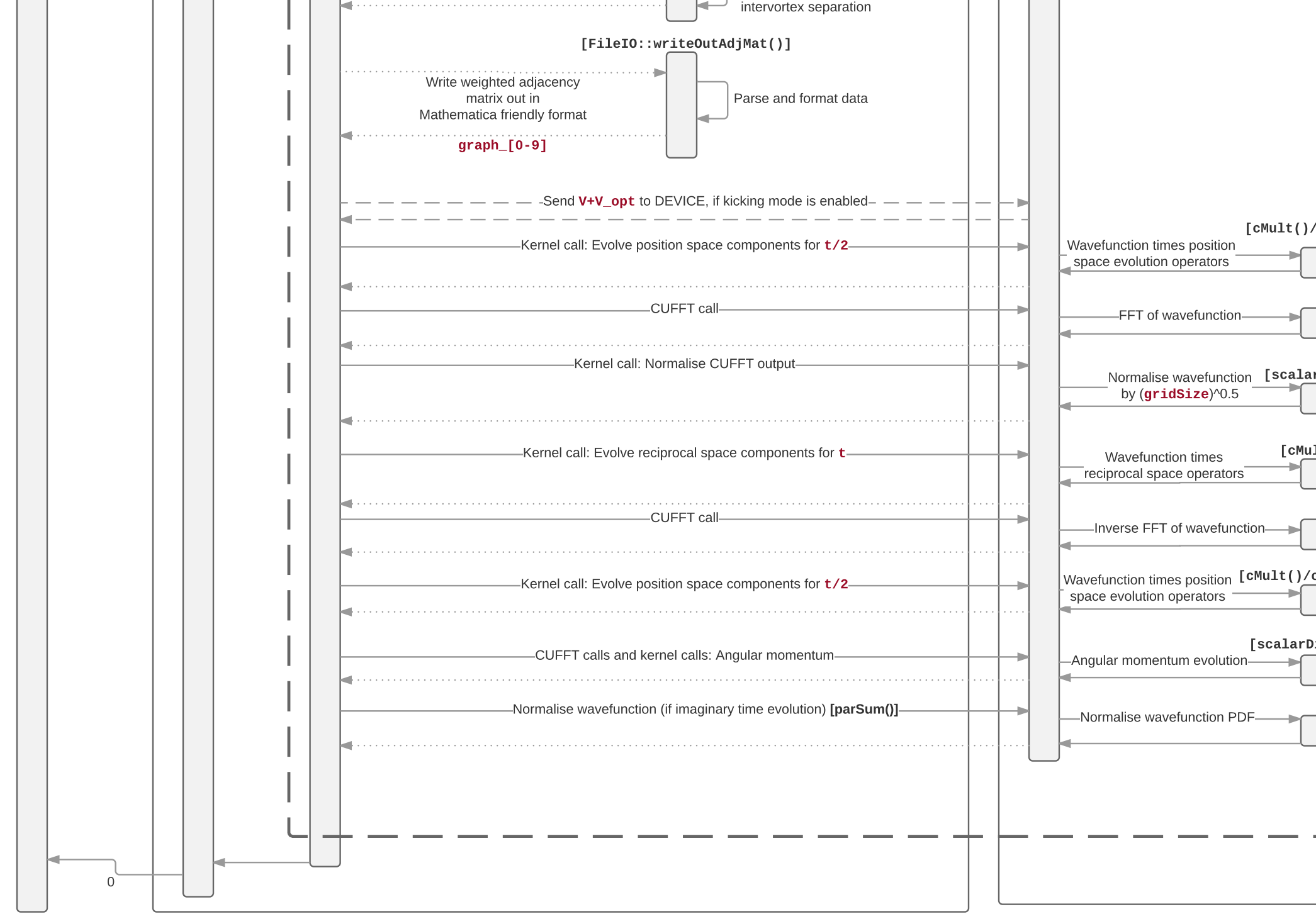
Find most
central vortex**central_vortex**





[cMultPhi()]





`mult()/cMultDensity()`



`[scalarDiv()]`



`[cMult()]`



`mult()/cMultDensity()`



`scalarDiv(), angularOp()`

